

EAST UPDATE 9/9/04, 466

L Number	Hits	Search Text	DB	Time stamp
1	10396	(pyrimidin or pyrimidinyl or pyrimidyl) and (sulfonamide or sulfonyl or sulfonamido)	USPAT; US-PGPUB	2004/03/24 14:21
2	2167	((pyrimidin or pyrimidinyl or pyrimidyl) and (sulfonamide or sulfonyl or sulfonamido)) and alanine	USPAT; US-PGPUB	2004/03/24 14:23

09/ 910,466

## Connecting via Winsock to STN

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LOGINID: ssspta1202txn

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

NEWS 1 Web Page URLs for STN Seminar Schedule - N. America  
NEWS 2 "Ask CAS" for self-help around the clock  
NEWS 3 SEP 09 CA/CAplus records now contain indexing from 1907 to the present  
NEWS 4 DEC 08 INPADOC: Legal Status data reloaded  
NEWS 5 SEP 29 DISSABS now available on STN  
NEWS 6 OCT 10 PCTFULL: Two new display fields added  
NEWS 7 OCT 21 BIOSIS file reloaded and enhanced  
NEWS 8 OCT 28 BIOSIS file segment of TOXCENTER reloaded and enhanced  
NEWS 9 NOV 24 MSDS-CCOHS file reloaded  
NEWS 10 DEC 08 CABA reloaded with left truncation  
NEWS 11 DEC 08 IMS file names changed  
NEWS 12 DEC 09 Experimental property data collected by CAS now available in REGISTRY  
NEWS 13 DEC 09 STN Entry Date available for display in REGISTRY and CA/CAplus  
NEWS 14 DEC 17 DGENE: Two new display fields added  
NEWS 15 DEC 18 BIOTECHNO no longer updated  
NEWS 16 DEC 19 CROPU no longer updated; subscriber discount no longer available  
NEWS 17 DEC 22 Additional INPI reactions and pre-1907 documents added to CAS databases  
NEWS 18 DEC 22 IFIPAT/IFIUDB/IFICDB reloaded with new data and search fields  
NEWS 19 DEC 22 ABI-INFORM now available on STN  
NEWS 20 JAN 27 Source of Registration (SR) information in REGISTRY updated and searchable  
NEWS 21 JAN 27 A new search aid, the Company Name Thesaurus, available in CA/CAplus  
NEWS 22 FEB 05 German (DE) application and patent publication number format changes  
NEWS 23 MAR 03 MEDLINE and LMEDLINE reloaded  
NEWS 24 MAR 03 MEDLINE file segment of TOXCENTER reloaded  
NEWS 25 MAR 03 FRANCEPAT now available on STN  
  
NEWS EXPRESS MARCH 5 CURRENT WINDOWS VERSION IS V7.00A, CURRENT MACINTOSH VERSION IS V6.0b(ENG) AND V6.0Jb(JP), AND CURRENT DISCOVER FILE IS DATED 3 MARCH 2004  
NEWS HOURS STN Operating Hours Plus Help Desk Availability  
NEWS INTER General Internet Information  
NEWS LOGIN Welcome Banner and News Items  
NEWS PHONE Direct Dial and Telecommunication Network Access to STN  
NEWS WWW CAS World Wide Web Site (general information)

Enter NEWS followed by the item number or name to see news on that specific topic.

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FILE 'HOME' ENTERED AT 15:00:11 ON 24 MAR 2004

FILE 'REGISTRY' ENTERED AT 15:00:20 ON 24 MAR 2004  
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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 23 MAR 2004 HIGHEST RN 666817-09-0  
DICTIONARY FILE UPDATES: 23 MAR 2004 HIGHEST RN 666817-09-0

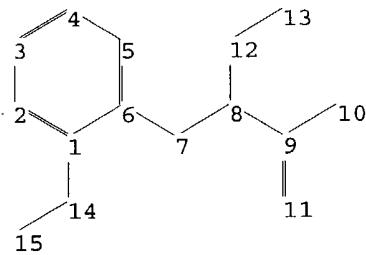
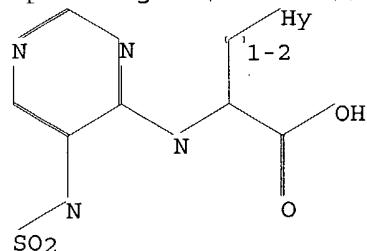
TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See **HELP CROSSOVER** for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:  
<http://www.cas.org/ONLINE/DBSS/reqistryss.html>

=>  
Uploading C:\STNEXP4\QUERIES\09910466a.str



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7 8 9 10 11 12 13 14 15  
ring nodes :  
1 2 3 4 5 6  
chain bonds :  
1-14 6-7 7-8 8-9 8-12 9-10 9-11 12-13 14-15  
ring bonds :  
1-2 1-6 2-3 3-4 4-5 5-6  
exact/norm bonds :  
1-14 6-7 7-8 12-13 14-15  
exact bonds :  
8-9 8-12  
normalized bonds :  
1-2 1-6 2-3 3-4 4-5 5-6 9-10 9-11
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09/ 910,466

isolated ring systems :  
containing 1 :

Match level :

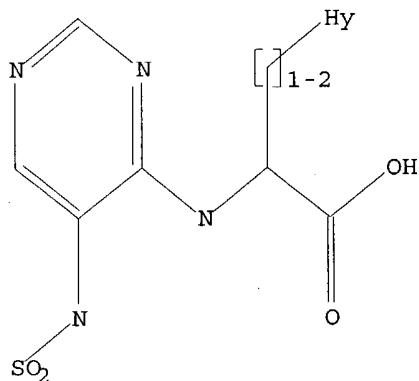
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS  
11:CLASS 12:CLASS 13:Atom 14:CLASS 15:CLASS

L1 STRUCTURE UPLOADED

=> d 11

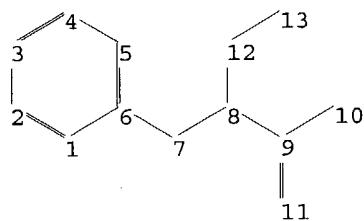
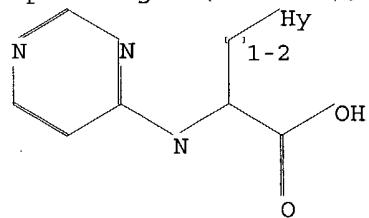
L1 HAS NO ANSWERS

L1 STR



Structure attributes must be viewed using STN Express query preparation.

=>  
Uploading C:\STNEXP4\QUERIES\09910466b.str



chain nodes :

7 8 9 10 11 12 13

ring nodes :

1 2 3 4 5 6

chain bonds :

6-7 7-8 8-9 8-12 9-10 9-11 12-13

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6

exact/norm bonds :

6-7 7-8 12-13

exact bonds :

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normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 9-10 9-11

isolated ring systems :

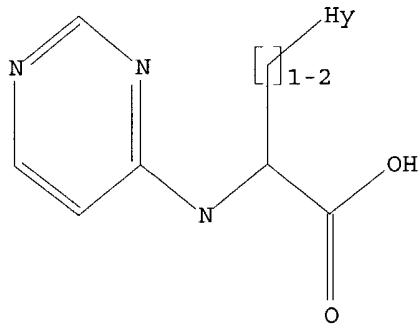
containing 1 :

09/ 910,466

Match level :  
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS  
11:CLASS 12:CLASS 13:Atom

L2 STRUCTURE UPLOADED

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L2 HAS NO ANSWERS  
L2 STR



Structure attributes must be viewed using STN Express query preparation.

=> s 11 ful  
FULL SEARCH INITIATED 15:01:00 FILE 'REGISTRY'  
FULL SCREEN SEARCH COMPLETED - 66 TO ITERATE

100.0% PROCESSED 66 ITERATIONS 0 ANSWERS  
SEARCH TIME: 00.00.01

L3 0 SEA SSS FUL L1

=> s 12 ful  
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FULL SCREEN SEARCH COMPLETED - 968 TO ITERATE

100.0% PROCESSED 968 ITERATIONS 16 ANSWERS  
SEARCH TIME: 00.00.01

L4 16 SEA SSS FUL L2

=> file caplus  
COST IN U.S. DOLLARS SINCE FILE TOTAL  
FULL ESTIMATED COST ENTRY SESSION  
310.42 310.63

FILE 'CAPLUS' ENTERED AT 15:01:13 ON 24 MAR 2004  
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.  
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FILE COVERS 1907 - 24 Mar 2004 VOL 140 ISS 13  
FILE LAST UPDATED: 23 Mar 2004 (20040323/ED)

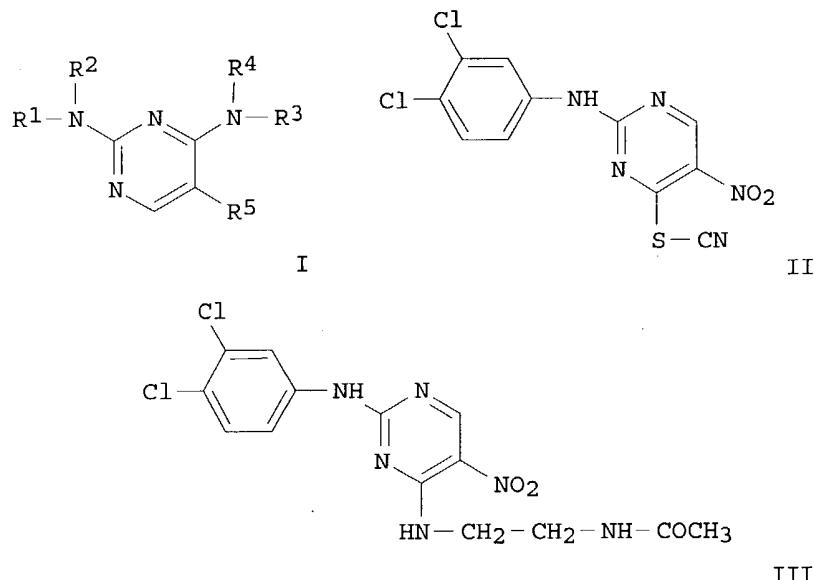
This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 14  
L5 13 L4

=> d 15 1- ibib abs hitstr  
YOU HAVE REQUESTED DATA FROM 13 ANSWERS - CONTINUE? Y/(N):y

L5 ANSWER 1 OF 13 CAPLUS COPYRIGHT 2004 ACS on STN  
ACCESSION NUMBER: 2003:319721 CAPLUS  
DOCUMENT NUMBER: 138:321292  
TITLE: Preparation of 2,4,5-trisubstituted pyrimidines as cyclin dependent kinase inhibitors  
INVENTOR(S): Dahmann, Georg; Himmelsbach, Frank; Wittneben, Helmut; Pautsch, Alexander; Prokopowicz, Anthony S.; Krist, Bernd; Schnapp, Gisela; Steegmaier, Martin; Lenter, Martin; Schoop, Andreas; Steurer, Steffen; Spevak, Walter  
PATENT ASSIGNEE(S): Boehringer Ingelheim Pharma K.-G., Germany; Boehringer Ingelheim Pharmaceuticals, Inc.; Boehringer Ingelheim International G.m.b.H.  
SOURCE: PCT Int. Appl., 278 pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent  
LANGUAGE: German  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003032997	A1	20030424	WO 2002-EP11453	20021014
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
US 2003171359	A1	20030911	US 2002-271763	20021016
PRIORITY APPLN. INFO.:			US 2001-330145P	P 20011017
OTHER SOURCE(S):		MARPAT 138:321292		
GI				



AB Title compds. I [R1 = H, alkyl; R2 = (un)substituted alkyl; R3 = H, alkyl; R4 = (un)substituted alkyl; R5 = halo] and their pharmaceutically acceptable salts were prepared. For example, condensation of thiocyanatopyrimide II, e.g., prepared from 3,4-dichloroaniline and 2-chloro-4-thiocyanato-5-nitropyrimidine in one step, and acetylaminooethylamine provided trisubstituted pyrimidine III in 88% yield. In CDK1/CyclinB1 kinase inhibition studies, 88-examples of compds. I exhibited IC<sub>50</sub> values more than 100 nM. Compds. I are claimed useful for the treatment of diseases characterized by abnormal cell proliferation.

IT 514831-25-5P, 2-(3,4-Dichlorophenylamino)-4-[(*1S*)-1-carboxy-2-(1*H*-imidazol-4-yl)ethyl]amino]-5-trifluoromethylpyrimidine

**514832-15-6P**, 2-[(3,4-Dichlorophenylamino)-4-[(1*R*)-1-camimidazol-4-yl]ethyl]amino]-5-trifluoromethylpyrimidine

514832-70-3P

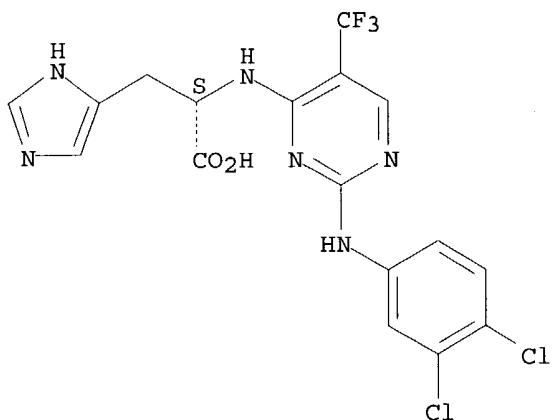
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; preparation of trisubstituted pyrimidines as cyclin dependent kinase inhibitors)

BN 514831-25-5 CAPLUS

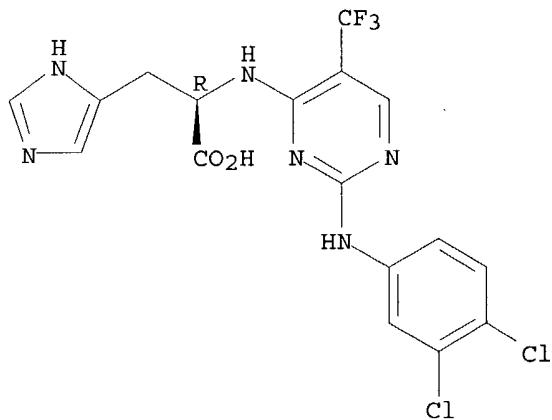
CN L-Histidine, N-[2-[(3,4-dichlorophenyl)amino]-5-(trifluoromethyl)-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

## Absolute stereochemistry.



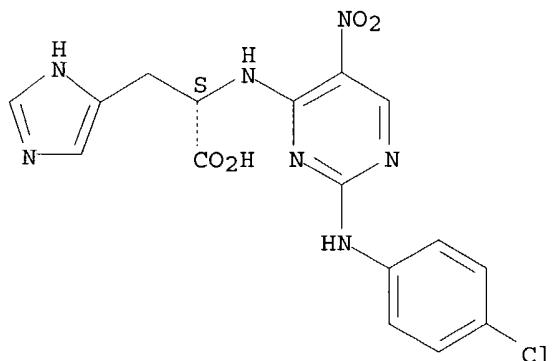
RN 514832-15-6 CAPLUS  
CN D-Histidine, N-[2-[(3,4-dichlorophenyl)amino]-5-(trifluoromethyl)-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 514832-70-3 CAPLUS  
CN L-Histidine, N-[2-[(4-chlorophenyl)amino]-5-nitro-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

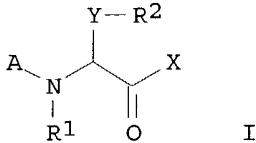
Absolute stereochemistry.



## RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 2 OF 13 CAPLUS COPYRIGHT 2004 ACS on STN  
 ACCESSION NUMBER: 2002:90023 CAPLUS  
 DOCUMENT NUMBER: 136:135018  
 TITLE: Preparation of 3-(heteroaryl) alanine derivatives as  
 inhibitors of leukocyte adhesion mediated by VLA-4  
 INVENTOR(S): Konradi, Andrei W.; Pleiss, Michael A.; Thorsett,  
 Eugene D.; Ashwell, Susan; Welmaker, Gregory S.;  
 Kreft, Anthony; Sarantakis, Dimitrios; Dressen, Darren  
 B.; Grant, Francine S.; Semko, Christopher; Xu,  
 Ying-Zi; Stappenbeck, Frank  
 PATENT ASSIGNEE(S): Elan Pharmaceuticals, Inc., USA; American Home  
 Products Corporation  
 SOURCE: PCT Int. Appl., 132 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002008203	A2	20020131	WO 2001-US23097	20010720
WO 2002008203	A3	20020523		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2002052375	A1	20020502	US 2001-910466	20010719
PRIORITY APPLN. INFO.:			US 2000-220131P	P 20000721
OTHER SOURCE(S):		MARPAT 136:135018		<i>Gregory versus</i>
GI				



AB 3-(Heteroaryl)alanine derivs. I [A = an (un)substituted aryl, heteroaryl, cycloalkyl, or heterocyclic group; R2 = a nitrogen containing (un)substituted, heteroaryl; Y = (CH2)m; m = 0 or 1; R1 = H, (un)substituted, alkyl, alkenyl, cycloalkyl, cycloalkenyl, aryl, heteroaryl, or heterocyclic; X = OH, (un)substituted alkoxy, alkenoxy, cycloalkoxy, cycloalkenoxy, aryloxy, heteroaryloxy, heterocyclyloxy, or NR3R3 [R3 = H, (un)substituted alkyl, alkenyl, cycloalkyl, aryl, heteroaryl, or heterocyclic]] were prepared as inhibitors of leukocyte adhesion mediated by VLA-4. Compds. I have binding affinity to VLA-4 as expressed by an IC50 of about 15  $\mu\text{M}$  or less. Thus, N-[5-(2,2,2-trifluoroethyl)pyrimidin-4-yl]-DL-3-[5-(2,5-dimethoxyphenyl)pyridin-2-yl]alanine was prepared by multistep procedure via coupling of DL-[5-(2,6-dimethoxyphenyl)pyridine-2-yl]alanine Et ester and 4,6-dichloro-5-(2,2,2-trifluoroethyl)pyrimidine.

IT 392298-39-4P 392298-40-7P 392298-42-9P  
 392298-43-0P

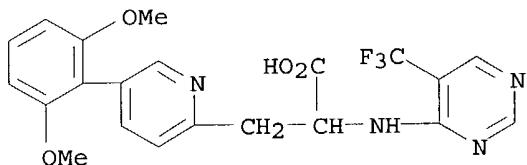
09/ 910,466

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of alanine derivs. as inhibitors of leukocyte adhesion mediated by VLA-4)

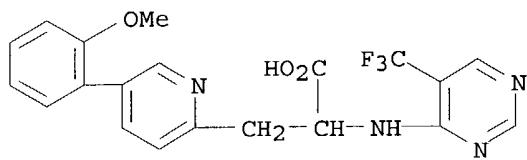
RN 392298-39-4 CAPLUS

CN 2-Pyridinepropanoic acid, 5-(2,6-dimethoxyphenyl)- $\alpha$ -[[5-(trifluoromethyl)-4-pyrimidinyl]amino]- (9CI) (CA INDEX NAME)



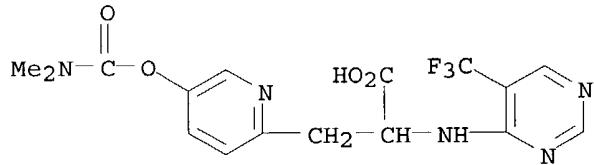
RN 392298-40-7 CAPLUS

CN 2-Pyridinepropanoic acid, 5-(2-methoxyphenyl)- $\alpha$ -[[5-(trifluoromethyl)-4-pyrimidinyl]amino]- (9CI) (CA INDEX NAME)



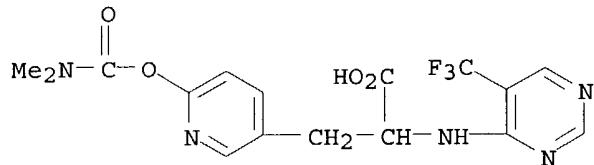
RN 392298-42-9 CAPLUS

CN 2-Pyridinepropanoic acid, 5-[[[(dimethylamino)carbonyl]oxy]- $\alpha$ -[[5-(trifluoromethyl)-4-pyrimidinyl]amino]- (9CI) (CA INDEX NAME)



RN 392298-43-0 CAPLUS

CN 3-Pyridinepropanoic acid, 6-[[[(dimethylamino)carbonyl]oxy]- $\alpha$ -[[5-(trifluoromethyl)-4-pyrimidinyl]amino]- (9CI) (CA INDEX NAME)



L5 ANSWER 3 OF 13 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2001:63992 CAPLUS

DOCUMENT NUMBER: 134:116237

TITLE: Preparation of bradykinin B1 receptor antagonists  
INVENTOR(S): Ohlmeyer, Michael H. J.; Baldwin, John J.; Dolle,

Roland E., III; Paradkar, Vidyadhar; Quintero, Jorge  
 Gabriel; Pan, Gonghua  
 PATENT ASSIGNEE(S) : Pharmacopeia, Inc., USA  
 SOURCE: PCT Int. Appl., 231 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001005783	A1	20010125	WO 2000-US19185	20000714
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
EP 1196411	A1	20020417	EP 2000-950343	20000714
EP 1196411	B1	20030917		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
JP 2003505384	T2	20030212	JP 2001-511442	20000714
AT 250053	E	20031015	AT 2000-950343	20000714
US 2003229092	A1	20031211	US 2002-46616	20020114
PRIORITY APPLN. INFO.:			US 1999-143990P	P 19990715
			WO 2000-US19185	W 20000714

OTHER SOURCE(S) : MARPAT 134:116237

GI

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB Compds. I [X, Y, Z = CH or N; A = A1 or A2, where A1 is R4R5NCO (R4 = H, aryl, heteroaryl, substituted alkyl; R5 = H, alkyl), 5-aryl-1,2,4-triazol-3-yl, 2-aryl-4-imidazolyl, or 2-aryl-5-thiazolyl and A2 is R7CONH (R7 = aryl or alkylaryl), R7SO2NH, R4NH, R4O; Q = heteroaryl, aryl, CH2R13 (R13 = OH, OTHP, 1-imidazolyl, 1-pyrrolyl), CH:NOMe, or 1,3-dithian-2-yl; W = H, Cl, F, alkyl, aryl, heteroaryl, alkoxy, alkylthio, an amino group, arylcarbamoyl, etc.; R1 = alkyl, cycloalkyl, heterocyclyl, aryl, heteroaryl, etc.; R2 = H or alkyl or R1R2C is a ring optionally containing O, S or N; R3 = H or alkyl, or when n is zero, R2 and R3 taken together form a 6-membered ring (with provisos)] were prepared as bradykinin B1 receptor antagonists. Thus, D-leucine derivative II was prepared by substitution reaction of D-leucine 4-chlorobenzylamide with 2,4-dichloro- (or difluoro)-6-(1H-imidazol-1-yl)pyrimidine and then 3-chlorobenzylamine. Pharmaceutical formulations containing II are described.

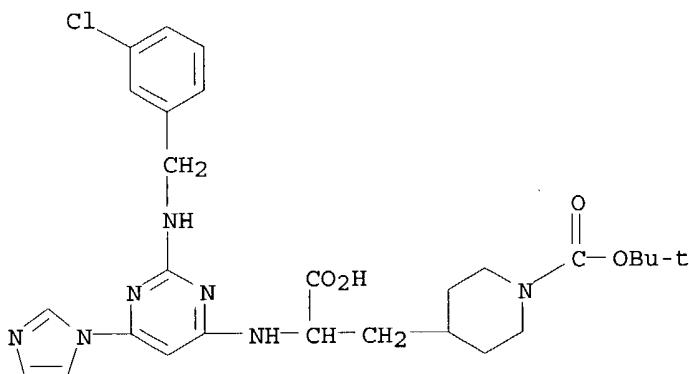
IT 321328-55-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of bradykinin B1 receptor antagonists)

RN 321328-55-6 CAPLUS

CN 4-Piperidinepropanoic acid,  $\alpha$ -[[2-[(3-chlorophenyl)methyl]amino]-6-(1H-imidazol-1-yl)-4-pyrimidinyl]amino]-1-[(1,1-dimethyllethoxy)carbonyl]-(9CI) (CA INDEX NAME)



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 4 OF 13 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1993:508382 CAPLUS

DOCUMENT NUMBER: 119:108382

TITLE: In vitro cytostatic activity of some amino acid 4-N-substituted cytosines

AUTHOR(S): Hladon, Boguslaw; Sloderbach, Anna; Radosh, Przemyslaw; Spychala, Jaroslaw; Golankiewicz, Krzysztof

CORPORATE SOURCE: Dep. Pharmacol., Med. Acad., Poznan, 61-701, Pol.

SOURCE: Archivum Immunologiae et Therapiae Experimentalis (1992), 40(2), 145-50

CODEN: AITEAT; ISSN: 0004-069X

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The cytotoxicity of 16 cytosine derivs. substituted at position N4 with amino acid and related moieties was studied on human carcinoma cells in vitro. The activity of the compds. was inversely related to their solubility. The most active compound, and the only one seemed suitable for further investigation, was N4-(1H-2-oxo-4-pyrimidinyl)tryptamine. Some hypothetical structure-activity relationships are briefly discussed.

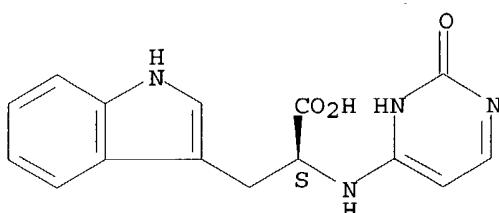
IT 93734-66-8

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)  
(cytostatic activity of, structure in relation to)

RN 93734-66-8 CAPLUS

CN L-Tryptophan, N-(1,2-dihydro-2-oxo-4-pyrimidinyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 5 OF 13 CAPLUS COPYRIGHT 2004 ACS on STN

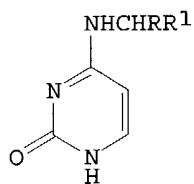
ACCESSION NUMBER: 1989:477735 CAPLUS

DOCUMENT NUMBER: 111:77735

TITLE: Photochemical synthesis of deuterium-labeled 4-N-substituted cytosines

09/ 910,466

AUTHOR(S): Celewicz, Lech; Spychala, Jaroslaw; Golankiewicz, Krzysztof  
CORPORATE SOURCE: Fac. Chem., Adam Mickiewicz Univ., Poznan, 60-780, Pol.  
SOURCE: Journal of Labelled Compounds and Radiopharmaceuticals (1988), 25(12), 1401-5  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
OTHER SOURCE(S): CASREACT 111:77735  
GI



I

AB Deuteroalkylcytosines I (R = D; R1 = H, Me, CHMe2, CH2OH, CH2CO2H, CH2Ph, 3-benzimidazolylmethyl) were obtained in 45-85% yield by photochem. decarboxylation of I (R = CO2H) in the presence of D2O or MeOD.

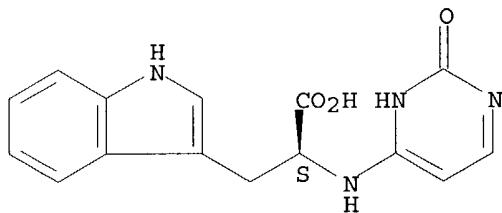
IT 93734-66-8

RL: RCT (Reactant); RACT (Reactant or reagent)  
(photochem. decarboxylation-deuteration of)

RN 93734-66-8 CAPLUS

CN L-Tryptophan, N-(1,2-dihydro-2-oxo-4-pyrimidinyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 6 OF 13 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1988:618460 CAPLUS

DOCUMENT NUMBER: 109:218460

TITLE: Intramolecular OH...N .dblharw. O-...H+N hydrogen bonds in N-(1H-2-oxo-4-pyrimidinyl) amino acids

AUTHOR(S): Brzezinski, Bogumil; Celewicz, Lech; Spychala, Jaroslaw; Golankiewicz, Krzysztof

CORPORATE SOURCE: Dep. Chem., Adam Mickiewicz Univ., Poznan, 60-780, Pol.

SOURCE: Chemical Physics Letters (1988), 149(4), 348-54  
DOCUMENT TYPE: Journal  
LANGUAGE: English

AB Seven N-(1H-2-oxo-4-pyrimidinyl) amino acids were studied by NMR and FTIR spectroscopy. In (CD3)2SO solns. easily polarizable intramol. OH...N .dblharw. O-...H+N bonds were formed and the IR continuum was observed. In aqueous solns. the intramol. H bonds were broken and the tautomeric equilibrium shifted towards the zwitterion.

09/ 910,466

IT 93734-66-8

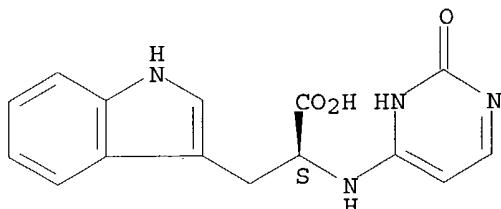
RL: PRP (Properties)

(IR and NMR spectra of, hydrogen bonds in relation to)

RN 93734-66-8 CAPLUS

CN L-Tryptophan, N-(1,2-dihydro-2-oxo-4-pyrimidinyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 7 OF 13 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1988:610774 CAPLUS

DOCUMENT NUMBER: 109:210774

TITLE: Photochemical synthesis of N4-substituted cytosines

AUTHOR(S): Celewicz, Lech; Spychala, Jaroslaw; Golankiewicz, Krzysztof

CORPORATE SOURCE: Fac. Chem., Adam Mickiewicz Univ., Poznan, 60-780, Pol.

SOURCE: Synthetic Communications (1987), 17(16), 1939-50

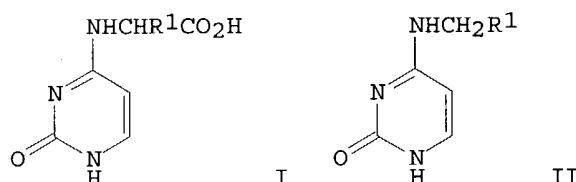
CODEN: SYNCV; ISSN: 0039-7911

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 109:210774

GI



AB Pyrimidinyl-substituted L-amino acids I [R<sub>1</sub> = H, Me, CH<sub>2</sub>CHMe<sub>2</sub>, CHMeEt, CH<sub>2</sub>OH, CH(OH)Me, CH<sub>2</sub>CO<sub>2</sub>H, CH<sub>2</sub>Ph, 3-indolylmethyl] underwent photochem. decarboxylation to give cytosines II. II [R<sub>1</sub> = CH<sub>2</sub>OH, CH(OH)Me] were irradiated to give II (R<sub>1</sub> = Me).

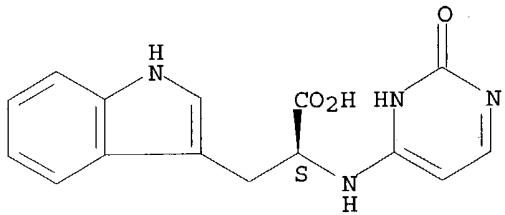
IT 93734-66-8

RL: RCT (Reactant); RACT (Reactant or reagent)  
(photochem. decarboxylation of)

RN 93734-66-8 CAPLUS

CN L-Tryptophan, N-(1,2-dihydro-2-oxo-4-pyrimidinyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 8 OF 13 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1975:422276 CAPLUS

DOCUMENT NUMBER: 83:22276

TITLE: Effect of some pyrimidine amino acid derivatives on  
vaccinia virus in tissue cultureAUTHOR(S): Izergina, E. A.; Votyakov, V. I.; Balandin, I. G.;  
Kabailova, I. V.; Seleznev, A. F.; Andreeva, O. T.;  
Lidak, M. Yu.CORPORATE SOURCE: Beloruss. Nauchno-Issled. Inst. Epidemiol.,  
Mikrobiol., Minsk, USSRSOURCE: Voprosy Virusologii (1975), (1), 51-4  
CODEN: VVIRAT; ISSN: 0507-4088DOCUMENT TYPE: Journal  
LANGUAGE: Russian

GI For diagram(s), see printed CA Issue.

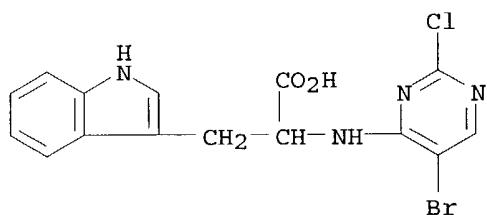
AB Of the 9 pyrimidine derivs. tested, only N-(2-chloro-5-bromo-4-pyrimidinyl)-DL-leucine (I) [35026-05-2] showed any antiviral activity against vaccinia viruses in chick embryo fibroblast culture. I inhibited DNA synthesis in the infected cultures, and decreased the infectious titer of the virus.

IT 35023-48-4

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)  
(virus response to, vaccinia)

RN 35023-48-4 CAPLUS

CN Tryptophan, N-(5-bromo-2-chloro-4-pyrimidinyl)- (9CI) (CA INDEX NAME)



L5 ANSWER 9 OF 13 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1972:25548 CAPLUS

DOCUMENT NUMBER: 76:25548

TITLE: Synthesis of N-(2-chloro-5-bromo-4-pyrimidyl)- and  
N-(2-chloro-5-iodo-4-pyrimidyl)amino acids

AUTHOR(S): Ulane, I.; Lidaks, M.

CORPORATE SOURCE: Inst. Org. Sint., Riga, USSR

SOURCE: Khimiya Geterotsiklicheskikh Soedinenii (1971), 7(4),  
527-9DOCUMENT TYPE: Journal  
LANGUAGE: Russian

CODEN: KGSSAQ; ISSN: 0132-6244

GI For diagram(s), see printed CA Issue.

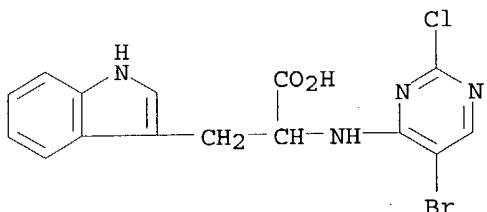
AB The title compds. (I, X = Br, R = DL-NHCHMeCO<sub>2</sub>H, DL-leucyl, L-leucyl, L-valyl, DL-methionyl, DL-tryptophanyl, L-isoleucyl, DL-glycyl; and X = I, R = L-leucyl, DL-leucyl, DL-valyl, DL-alanyl) were prepared in 31-50% yield, (from either 2,4-dichloro-5-bromo- or -5-iodopyrimidine and the amino acid Na salt refluxed in H<sub>2</sub>O in 1:0.5 molar ratio) for their biol. evaluation as inhibitors of protein biosynthesis.

IT 35023-48-4P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 35023-48-4 CAPLUS

CN Tryptophan, N-(5-bromo-2-chloro-4-pyrimidinyl)- (9CI) (CA INDEX NAME)



L5 ANSWER 10 OF 13 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1971:449531 CAPLUS

DOCUMENT NUMBER: 75:49531

TITLE: Synthesis and properties of N-(2-chloro-5-fluoro-4-pyrimidyl)- and N-(2-ethylthio-5-fluoro-4-pyrimidyl) amino acids

AUTHOR(S): Paegle, R.; Plata, M.; Lidaks, M.; Popelis, J.

CORPORATE SOURCE: Inst. Org. Sint., Riga, USSR

SOURCE: Khimiya Geterotsiklichesikh Soedinenii (1971), 7(2), 258-61

CODEN: KGSSAQ; ISSN: 0132-6244

DOCUMENT TYPE: Journal

LANGUAGE: Russian

GI For diagram(s), see printed CA Issue.

AB The reaction of 2,4-dichloro-5-fluoropyrimidine or 2-(ethylthio)-4-chloro-5-fluoropyrimidine with amino acid sodium salts gave the title compds. (I, R = Cl, EtS; R<sub>1</sub> = NHCH<sub>2</sub>CO<sub>2</sub>H, NHCH(CO<sub>2</sub>H)CH<sub>2</sub>Ph, NHCH(CO<sub>2</sub>H)CH<sub>2</sub>CH<sub>2</sub>SMe, NHCH(CO<sub>2</sub>H)CHMe, NHCH(CO<sub>2</sub>H)CH<sub>2</sub>CHMe<sub>2</sub>, NHCH(CO<sub>2</sub>H)CH<sub>2</sub>(NC<sub>8</sub>H<sub>6</sub>, = 3-indolyl) and NHCH<sub>2</sub>CH<sub>2</sub>CO<sub>2</sub>H).

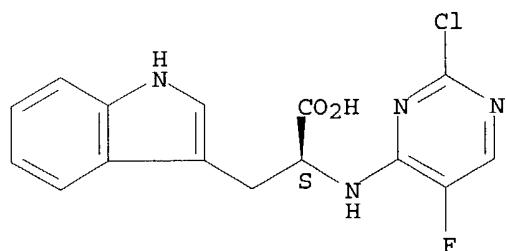
IT 34697-13-7P 34697-14-8P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 34697-13-7 CAPLUS

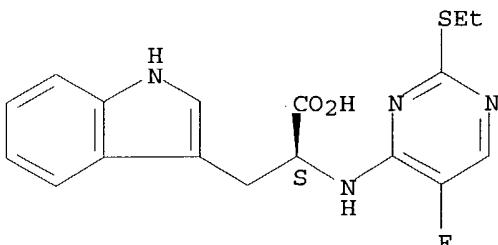
CN Tryptophan, N-(2-chloro-5-fluoro-4-pyrimidinyl)-, L- (8CI) (CA INDEX NAME)

Absolute stereochemistry.

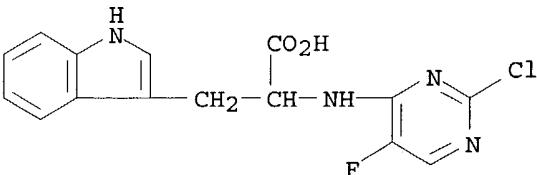


RN 34697-14-8 CAPLUS  
 CN Tryptophan, N-[2-(ethylthio)-5-fluoro-4-pyrimidinyl]-, L- (8CI) (CA INDEX  
 NAME)

Absolute stereochemistry.



L5 ANSWER 11 OF 13 CAPLUS COPYRIGHT 2004 ACS on STN  
 ACCESSION NUMBER: 1966:448006 CAPLUS  
 DOCUMENT NUMBER: 65:48006  
 ORIGINAL REFERENCE NO.: 65:9010f-h  
 TITLE: N-(2-Chloro-5-fluoro-4-pyrimidinyl)amino acids  
 AUTHOR(S): Paegle, R.; Plata, M.; Lidaks, M.  
 CORPORATE SOURCE: Inst. Org. Syn., Riga  
 SOURCE: Khimiya Geterotsiklichesikh Soedinenii (1966), (3),  
 475-6  
 CODEN: KGSSAQ; ISSN: 0132-6244  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Russian  
 GI For diagram(s), see printed CA Issue.  
 AB The N-(2-chloro-5-fluoro-4-pyrimidinyl)amino acids (I-VII) obtained from the reaction of 2,4-dichloro-5-fluorouracil with the appropriate amino acids. Me<sub>2</sub>CHOH-NH<sub>4</sub>OH-H<sub>2</sub>O; %, BuOH-HOAc-K<sub>2</sub>O; R, M.p., Yield, 9:1:1, 4:1:5, 14:1:5; I, H, 169°, 85, 0.87, -, 0.71; II, Me<sub>2</sub>CH, 179°, 80, -, 0.85, 0.90; III, Me<sub>2</sub>CHCH<sub>2</sub>, 173°, 84, -, 0.94, 0.86; IV, MeSCH<sub>2</sub>CH<sub>2</sub>, 159°, 66, -, 0.93, 0.81; V, PhCH<sub>2</sub>, 171°, 79, -, 0.93, 0.80; VI, 182°, 61, -, 0.90, 0.77; VII, 132°, 52, -, 0.88, 0.73;  
 IT 7662-32-0, Tryptophan, N-(2-chloro-5-fluoro-4-pyrimidinyl)-  
 (preparation of)  
 RN 7662-32-0 CAPLUS  
 CN Tryptophan, N-(2-chloro-5-fluoro-4-pyrimidinyl)- (7CI, 8CI) (CA INDEX  
 NAME)



L5 ANSWER 12 OF 13 CAPLUS COPYRIGHT 2004 ACS on STN  
 ACCESSION NUMBER: 1966:448005 CAPLUS  
 DOCUMENT NUMBER: 65:48005  
 ORIGINAL REFERENCE NO.: 65:9010d-f  
 TITLE: N-(2-Ethylthio-5-fluoro-4-pyrimidinyl)amino acids  
 AUTHOR(S): Paegle, R.; Plata, M.; Lidaks, M.  
 CORPORATE SOURCE: Inst. Org. Syn., Riga

SOURCE: Khimiya Geterotsiklicheskikh Soedinenii (1966), (3),  
474-5  
CODEN: KGSSAQ; ISSN: 0132-6244

DOCUMENT TYPE: Journal  
LANGUAGE: Russian

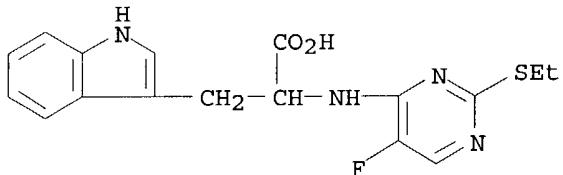
GI For diagram(s), see printed CA Issue.

AB The N-(2-ethylthio-5-fluoro-4-pyrimidinyl)amino acids (I-VII) were obtained from the reaction of 2-ethylthio-4-chloro-5-flourouracil with the appropriate amino acids. Rf;Me2CHOHNH4OH2O;%,BuOH-HOAc-H2O; R, M.p., Yield, 4:1:5, 9:1:1, 14:1:5; I, H, 215°, 70, -, -, 0.88; II, iso-Pr, 174°, 45, -, 0.85, 0.82; III, iso-Bu, 177°, 73, 0.95, -, 0.86; IV, MeSCH2CH2, 173°, 62, -, 0.84, 0.90; V, PhCH2, 186°, 67, -, 0.85, 0.92; VI, A, 198°, 69, 0.94, -, 0.87; VII, -, 141°, 52, 0.89, -, 0.90;

IT 7662-64-8, Tryptophan, N-[2-(ethylthio)-5-fluoro-4-pyrimidinyl]- (preparation of)

RN 7662-64-8 CAPLUS

CN Tryptophan, N-[2-(ethylthio)-5-fluoro-4-pyrimidinyl]- (7CI, 8CI) (CA INDEX NAME)



L5 ANSWER 13 OF 13 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1963:482495 CAPLUS  
DOCUMENT NUMBER: 59:82495  
ORIGINAL REFERENCE NO.: 59:15376h,15377a-b  
TITLE: Pyrimidine nucleosides. XVII. Pyrimidinyl amino acids  
AUTHOR(S): Ueda, Tohru; Fox, Jack J.  
CORPORATE SOURCE: Cornell Univ. Med. Coll., New York, NY  
SOURCE: Journal of Medicinal Chemistry (1963), 6(6), 697-701  
CODEN: JMCMAR; ISSN: 0022-2623

DOCUMENT TYPE: Journal  
LANGUAGE: Unavailable  
OTHER SOURCE(S): CASREACT 59:82495  
GI For diagram(s), see printed CA Issue.

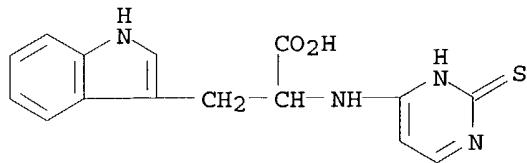
AB cf. CA 58, 11457a. N-(2-Oxo-4-pyrimidinyl) amino acids were prepared by reaction of 4-methylthio-2-pyrimidinones with amino acids. N-(2Oxo-4-pyrimidinyl)glycine, -L-alanine, -L-phenylalanine (I), -L-tryptophan (II), -β-alanine, -o- and p-amiobenzoic acid (III), and -glycylglycine were obtained. N-(2-Thio-4-pyrimidinyl)-L-tryptophan was also prepared as well as the 5-methyl, 5-fluoro (IV), 5-chloro, and 5-bromo analogs of N-(2-oxo-4-pyrimidinyl)-DL-alanine. The ribonucleosides of I, II, and III were synthesized by treatment of 1-β-D-ribofuranosyl-4-methylthio-2-pyrimidinone with the appropriate amino acid. The 1-(2-deoxy-β-D-ribofuranosyl) derivative of IV was synthesized by similar methods. Preliminary results with some of these compds. in exptl. tumors showed no significant antitumor activity. None of the pyrimidinyl amino acids tested supported the growth of certain pyrimidine- or amino acid-requiring mutants of *Escherichia coli*.

IT 93734-56-6, Tryptophan, N-(1,2-dihydro-2-thioxo-4-pyrimidinyl)-  
93734-66-8, Tryptophan, N-(1,2-dihydro-2-oxo-4-pyrimidinyl)- (preparation of)

RN 93734-56-6 CAPLUS

CN Tryptophan, N-(1,2-dihydro-2-thioxo-4-pyrimidinyl)- (7CI) (CA INDEX NAME)

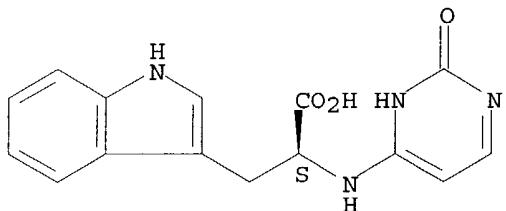
09/ 910,466



RN 93734-66-8 CAPLUS

CN L-Tryptophan, N-(1,2-dihydro-2-oxo-4-pyrimidinyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



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FILE 'REGISTRY' ENTERED AT 15:00:20 ON 24 MAR 2004

L1 STRUCTURE uploaded  
L2 STRUCTURE uploaded  
L3 0 S L1 FUL  
L4 16 S L2 FUL

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L5 13 S L4

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